Indian J. Phys. **69A** (1), 191 – 197 (1995)

I J P A
- an international journal

Effect of nonscattered modes on energy transport in one dimensional harmonic chain

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Abstract : We study the spatial evaluation of a localized energy pulse in one dimensional perfect as well as mass disordered (uncorrelated and correlated) harmonic chains. In the classical case the behavior of second moment ($M_2(t)$) of energy distribution strongly depends on the initial excitations, specially in disordered systems. Two types of initial excitations are considered here, namely (a) impulse excitation and (b) displacement excitation. The excitation is applied at a particular mass of the chain. We have shown that $M_2(t)$ can be expressed in terms of velocity-velocity correlation function in the case of impulse excitation. On the otherhand, it is energy current-energy current correlation function for the displacement excitation. The origin of these results has been shown to appear due to the different kinds of initial occupation probability of the modes of the system. For perfect harmonic chain the difference is seen at the amplitude of $M_2(t)$. On the otherhand, the effect is observed in the time exponent of $M_2(t)$ in disordered systems. Our numerical calculations also support the analytical results.

Keywords : Disordered solid, Energy transport
PACS Nos. : 61.43.j, 66.10.Cb

1 Introduction

Several unusual features have been recently observed [1] in amorphous systems. For example, thermal conductivity shows quadratic temperature dependence at low temperature, plateau at the intermediate temperature and further increase at higher temperature [1]. The behavior of the thermal conductivity from the plateau to the high temperature region appears to be understood by disorder and anharmonicity [2]. It is, therefore, essential to study the effect of disorder in the transport of energy. This consideration leads us to study here different kinds of uncorrelated and correlated disordered harmonic chains [3]. Recently, efforts have been directed to explain the unexpected features of amorphous systems by studying the spatial evaluation of a localized energy pulse and second moment of energy distribution [4, 5]. The interesting feature of the second moment is that it exhibits different behavior for different kinds of initial excitations, specially in disordered system. Two types of initial conditions are considered here, namely, (a) impulse excitation and (b) displacement excitation. They are given at a particular mass of the system. In earlier works [4, 5] the origin of this feature, however, has not been traced. The understanding of the behavior of the second moment for the two types of initial excitations is a further motivation behind this work. Our work is completely done in Fourier space, whereas, this type of calculation is invariably done in real space [4, 5]. To the best of our knowledge we show here for the first time that such a calculation can be done in the Fourier space without using directly the properties of Bessel functions.

2 Second moment of perfect chain

We consider here a one dimensional perfect and infinite harmonic chain consisting of masses M and springs with spring constant f. The Hamiltonian $\tilde{H}$ for this system is

$$\tilde{H} = \sum \tilde{h}_m(t) \tag{1}$$

and $\tilde{h}_m(t) = \tilde{P}_m^2/M + \frac{1}{4}\left[(Q_{m+1} - Q_m)^2 + (Q_m - Q_{m-1})^2\right]$. Here $\tilde{P}_m$ and Q_m define the momentum and the displacement respectively of the mass at the mth site. We now define

$$\omega^2 = f/M, \quad P_m = \tilde{P}_m/M\omega, \quad \tau = \omega t$$
$$h_m(t) = \tilde{h}_m(t)/M\omega^2, \quad H = \tilde{H}/M\omega^2, \quad J_m = Q_m - Q_{m-1}.$$

The quantity $h_m(\tau)/H$ gives the fraction of energy that resides at the m-th site at time τ. Consequently, it can be interpreted as the probability measure of a localized energy packet of unit strength to be found at the site m at time τ. So, the second moment of the energy distribution, $M_2(\tau)$ is defined as $M_2(\tau) = \sum_m m^2 h_m(\tau)/H$, where the initial excitation is introduced at the 0th mass. The second moment attains a status similar to the mean square displacement of an electron in a crystal. We solve the equations of motion for $P_m(\tau)$ and $J_m(\tau)$ in Fourier space and conequently we obtain the expressions of second moment $M_2(\tau)$ for two different types of initial conditions. The impulse excitation initially is given at the mass at site $n = 0$ i.e., $P_n(0) = \delta_{n,0}/M\omega$ and $Q_n(0) = 0$ for all n. We then obtain

$$\lim_{\tau\to\infty} M_2(\tau) = \frac{\tau^2}{2\pi}\int_{-\pi}^{\pi}\left(\frac{\partial\Omega}{\partial k}\right)^2 dk = \tau^2/2. \tag{2}$$

where, $\Omega^2(k) = 4\sin^2(k/2)$. On the otherhand, in the case of displacement excitation the initial conditions are $P_n(0) = 0$ and $Q_n(0) = \delta_{n,0}$. These initial conditions in turn yields

$$\lim_{\tau\to\infty} M_2(\tau) = \frac{\tau^2}{4\pi}\int_{-\pi}^{\pi}\left(\Omega\frac{\partial\Omega}{\partial k}\right)^2 dk = \tau^2/4. \tag{3}$$

Although in both cases, $M_2(\tau)$ shows the same time exponent, it is worthwhile to note that the amplitude differes by a factor of 2. The group velocity of this phonon wave packet $v_k = \partial\Omega/\partial k$. Hence, $M_2(\tau)$ is simply the phonon velocity-phonon velocity correlation function. In the case of displacement excitation, eq. (3) is treated as energy current-energy current correlation function. It can be easily shown that both the expression (2) and (3) can be obtained from the standard definition of velocity-velocity autocorrelation function. The difference arises because of the different kinds of initial

occupation probability $(h_k(0)/H)$. For the case of impulse excitation the initial occupation probability of all the modes are equal and it is $1/N$. On the otherhand, in the case of displacement excitation the initial occupation probability of the modes depends on k through $\Omega_k^2/2N$. The relevance of this discussion will be transparent in the subsequent sections where we discuss the behavior of $M_2(\tau)$ in the totally disordered and correlated disordered system.

3 The behavior of $M_2(\tau)$ in uncorrelated and correlated disordered harmonic chains

We first consider the uncorrelated mass disordered harmonic chain composed of mass m_p, with say $m_p = 1$ and m_d. The spring constant f is considered to be unity in all cases discussed below. Since disorder in the mass disordered harmonic chain vanishes at $\Omega = 0$, it has been shown that the system sustains $\sim \sqrt{N}$ nonscattered modes in the neighborhood of the zero frequency mode [6]. N defines the size of the sample. The number of nonscattered modes around zero frequency can be increased by introducing the correlation among masses. For example, consider a binarry system composed of masses m_p and a symmetric trimeric mass system. The central mass of this trimer is m_0 and other two masses are m_s. When $m_0 = 3 - 2m_s$ and $0 < m_s < 3/2$, a doubly degenerate reflectionless mode is obtained at $\Omega = 0$. In this case the number of nonscattered modes around zero frequency is $\sim N^{5/6}$ [3]. We employ here the DKP formula [7] to calculate the asymptotic behavior of $M_2(\tau)$ in time, τ for the two different initial conditions.

(a) Impulse excitation

Suppose the width of the nonscatered modes in the reciprocal space, $\Delta k \sim N^{-\beta}$ and $\beta > 0$. As the nonscattered modes are responsible for the energy transport we integrate the eq. (2) within the region Δk. Then according to DKP we obtain

$$M_2(\tau) \sim \frac{\tau^2}{2\pi} \int_0^{k_{max}} \left(\frac{\partial \Omega}{\partial k}\right)^2 dk = \frac{\tau^2}{2\pi} \Delta k. \tag{4}$$

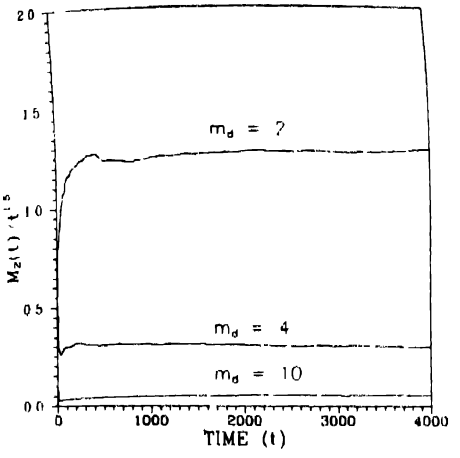

Figure 1. Plot of $M_2(t)/t^{1.5}$ with time t for uncorrelated mass disordered harmonic chains with the initially given impulse excitation.

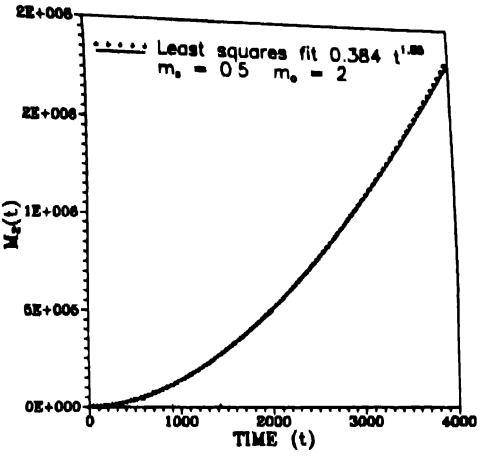

Figure 2. Plot of $M_2(t)$ as a function of t for symmetric trimer chain with degenerate resonances at $\Omega = 0$ with the initially given impulse excitation.

Furthermore, as group velocity v is $\sim$ unity around zero frequency, we obtain $N \sim \tau$. Since for completely disordered harmonic chain $\beta = 1/2$, $M_2(\tau) \sim \tau^{3/2}/2\pi$. In the case of symmetric random trimer chain with degenerate resonances we have $\beta = 1/6$. Hence, from the formula (4) we obtain $M_2(\tau) \sim \tau^{11/6}/2\pi$. The values of the exponents in numerical calculations (figure 1 and figure 2) are in excellent agreement with our analytical results.

(b) Displacement Excitation

Applying the same procedure to eq. (3), we obtain

$$M_2(\tau) \sim \frac{\tau^2}{4\pi} \int_0^{k_{max}} \sin^2 k \, dk = \frac{\tau^2}{12\pi} (\Delta k)^3. \tag{5}$$

For completely random system the eq. (5) gives $M_2(\tau) \sim \tau^{1/2}/12\pi$. On the otherhand for the symmetric trimer model with degenerate resonances at $\Omega = 0$, we obtain $M_2(\tau) \sim \tau^{1.5}/12\pi$. Some of our prototype results of numerical calculations are shown in figure 3 and figure 4. In the case of uncorrelated mass disordered chain we observe the oscillating behavior in $M_2(t)$ as well as the increasing tendency with time t. We fitted the plots with the

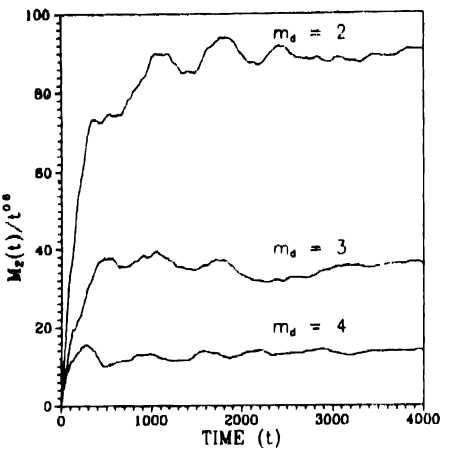

Figure 3. Plot of $M_2(t)/t^{0.6}$ against t for uncorrelated mass disordered harmonic chains with the initially given displacement excitation.

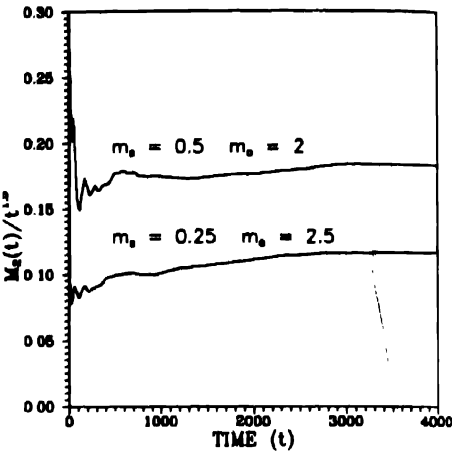

Figure 4. Plot of $M_2(t)/t^{1.5}$ as a function t for symmetric trimer chain with degenerate resonances at $\Omega = 0$ with the initially given displacement excitation.

exponent 0.6 of time t. The exponents in this case however, is significantly larger than the expected value (0.5). The spectrum of the complete disordered system contains many fringe resonances around zero frequency. The position of these resonances depends on the sample length as well as on the sample. Since all the nonscattered modes have equal occupation probability as $(1/N)$ in the case of momentum excitation they contribute equally to $M_2(t)$. On the otherhand, for displacement excitation the occupation probability of the nonscattered modes is given by $\Omega^2(k)/2N$. So, the contribution of these modes to $M_2(t)$ is weighted by $\Omega(k)$. Consequently, the fringe resonances contribute significantly to $M_2(t)$. The fluctuation occurs because fringe resonances appear randomly. To prove this we studied $M_2(t)$ with the displacement excitation of the symmetric random trimer model with dgenerate resonances at $\Omega = 0$ (figure 4). The expected value of the exponent is 1.5. The observed value agrees well with the prediction. Furthermore, the evoluation of $M_2(t)$ does not show any perceptible fluctuation. This is obtained because the width of the nonscattered modes is large comparative

to that in the uncorrelated disordered system. Hence, the contribution from the fringe resonances is suppressed.

4 Conclusion

The main features of this study are :

1) The second moment, $M_2(t)$ shows velocity-velocity correlation for impulse excitation and energy current-energy current correlation for displacement excitation. However, both the expression originally come from the velocity-velocity autocorrelation function. The disimilarity arises due to different kinds of initial occupation probability of the modes of the system. For impulse excitation the ocupation probability is $1/N$, whereas it is $\Omega_k^2/2N$ for displacement excitation.

2) The time exponent of $M_2(t)$ in disordered systems also depends on the correlation and the initial occupation probability of the modes in the system.

3) So, the correlation and the initial occupation probability of the modes can be used as control parameter in the study of low temperature thermal conductivity of amorphous materials.

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